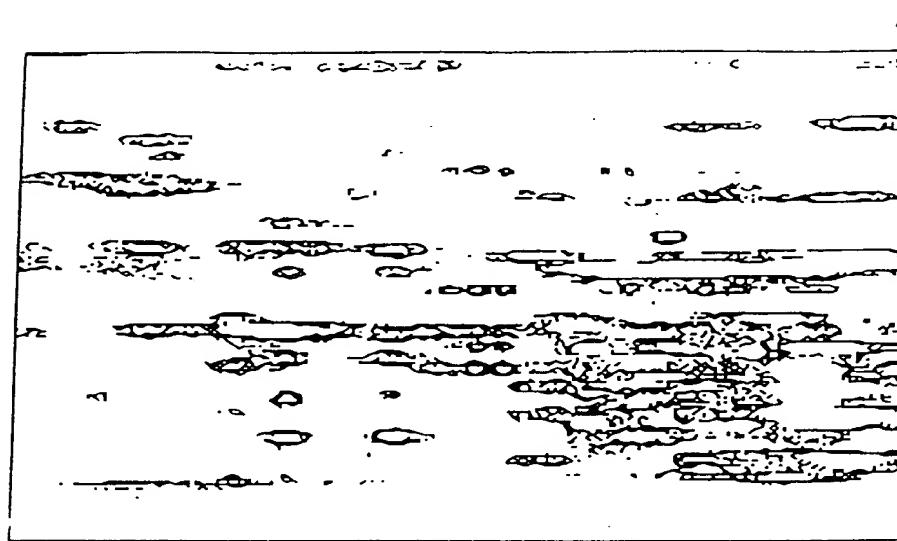


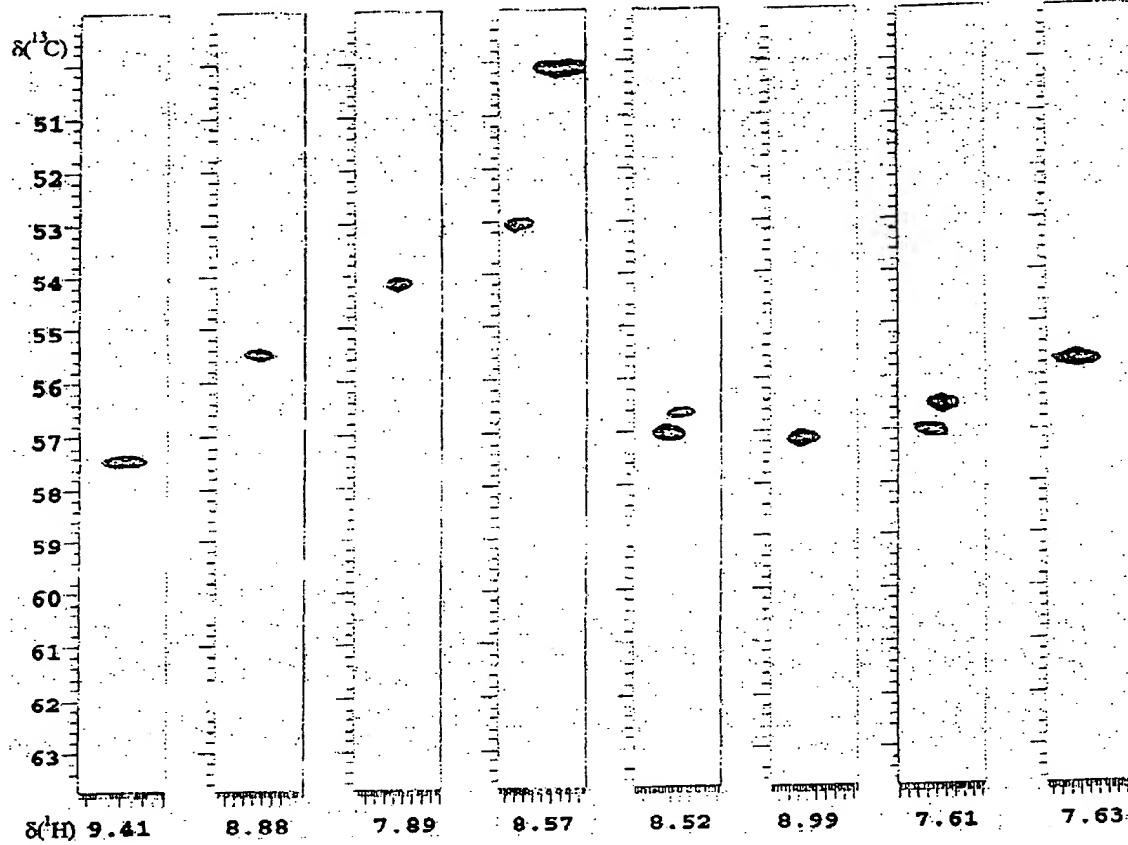
FIGURE 1A



2025 RELEASE UNDER E.O. 14176

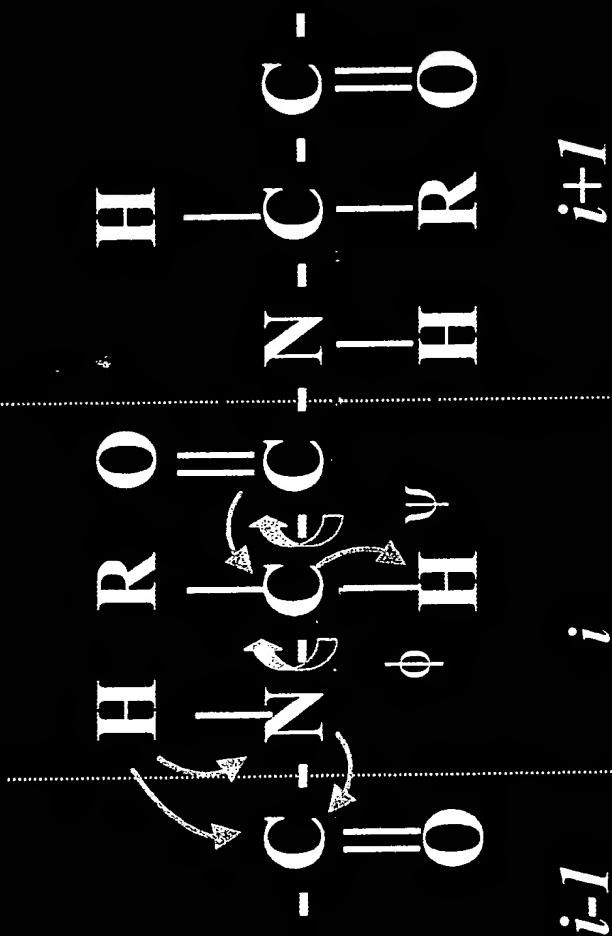
FIGURE 1B

10220T-02028660



B  
FIGURE 2

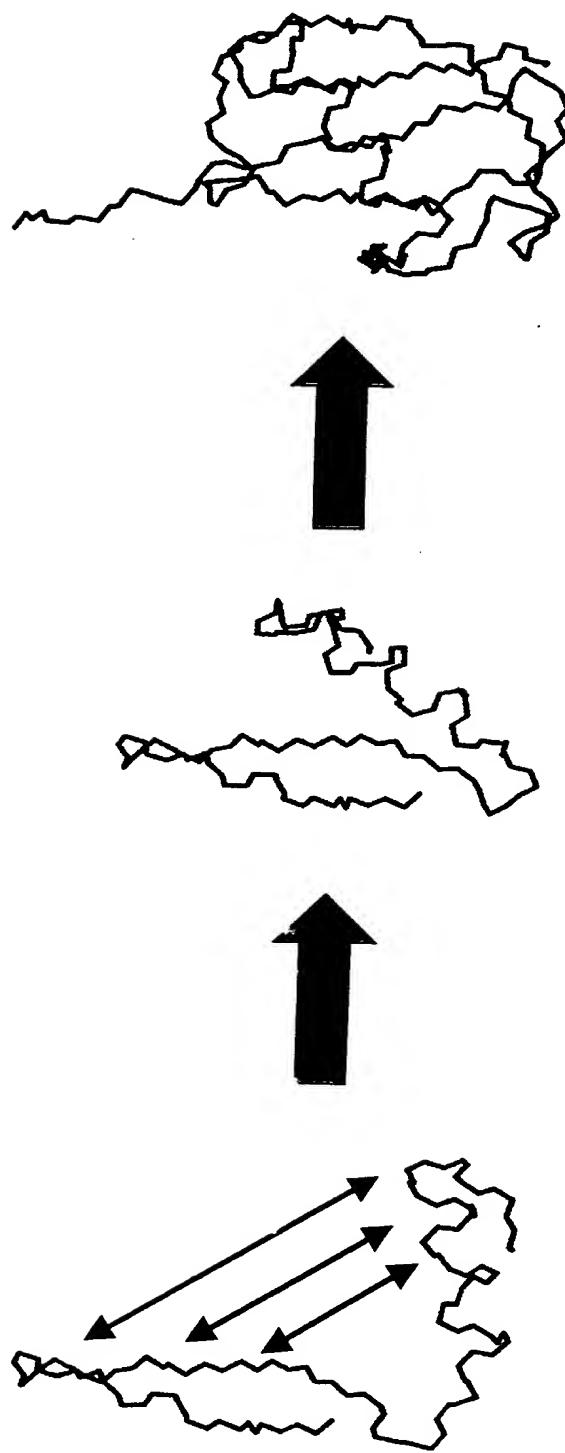
## Dipolar Couplings That Depend Only on $\phi(i)$ and $\psi(i)$



Search  $\phi$  and  $\psi$  Until Measured Couplings = Theoretical Couplings

# Packing Secondary Structural Elements

FIGURE 3



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RAPID DETERMINATION OF PROTEIN...  
Atty. Dkt. No. 1496-205  
Figure 3 of 13

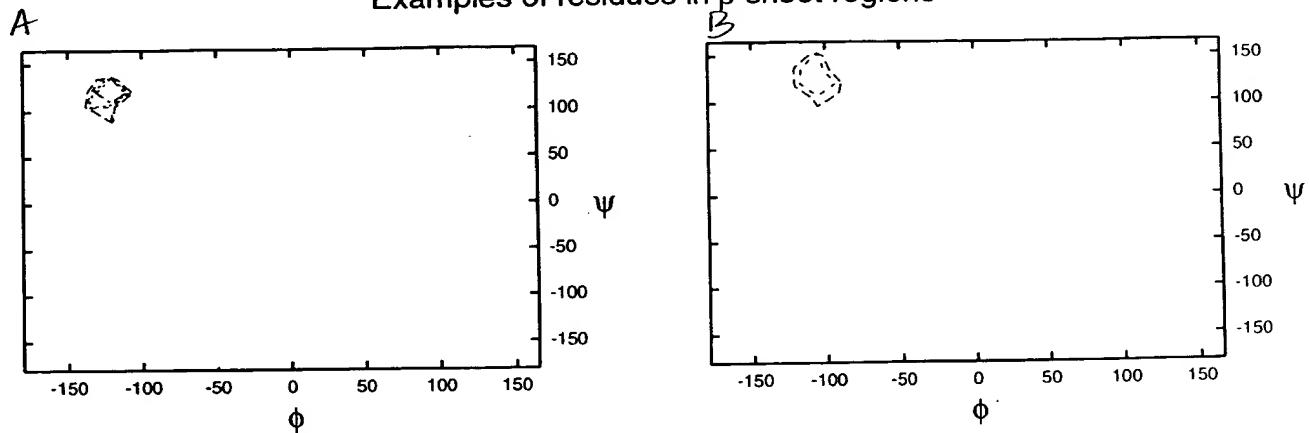
Final Structure

Packing Elements

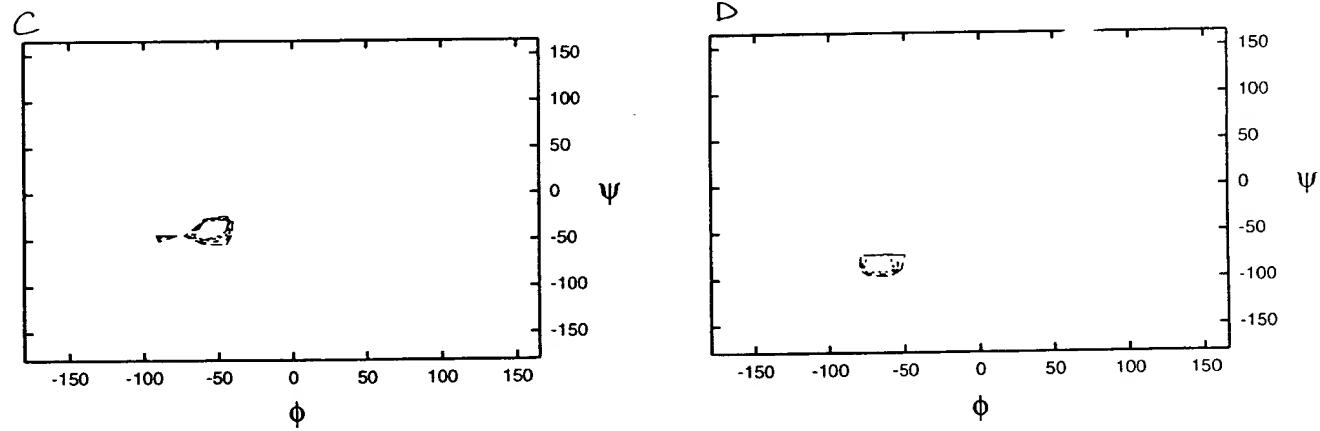
Long-range  $^1\text{H}$ - $^1\text{H}$  NOEs  
and Dipolar Couplings

FIGURE 4

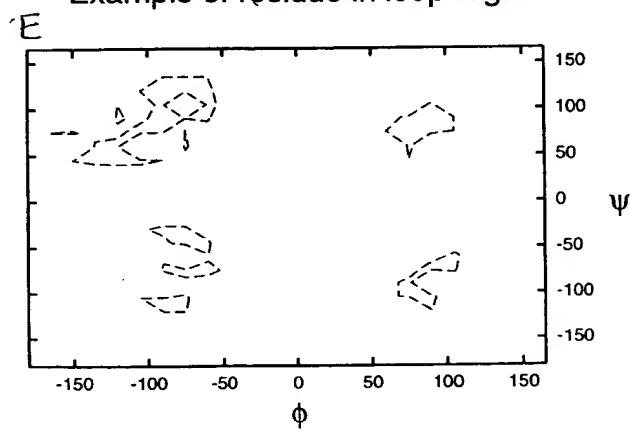
Examples of residues in  $\beta$ -sheet regions



Examples of residues in  $\alpha$ -helix regions



Example of residue in loop region



RECEIVED DEPT OF POLICE

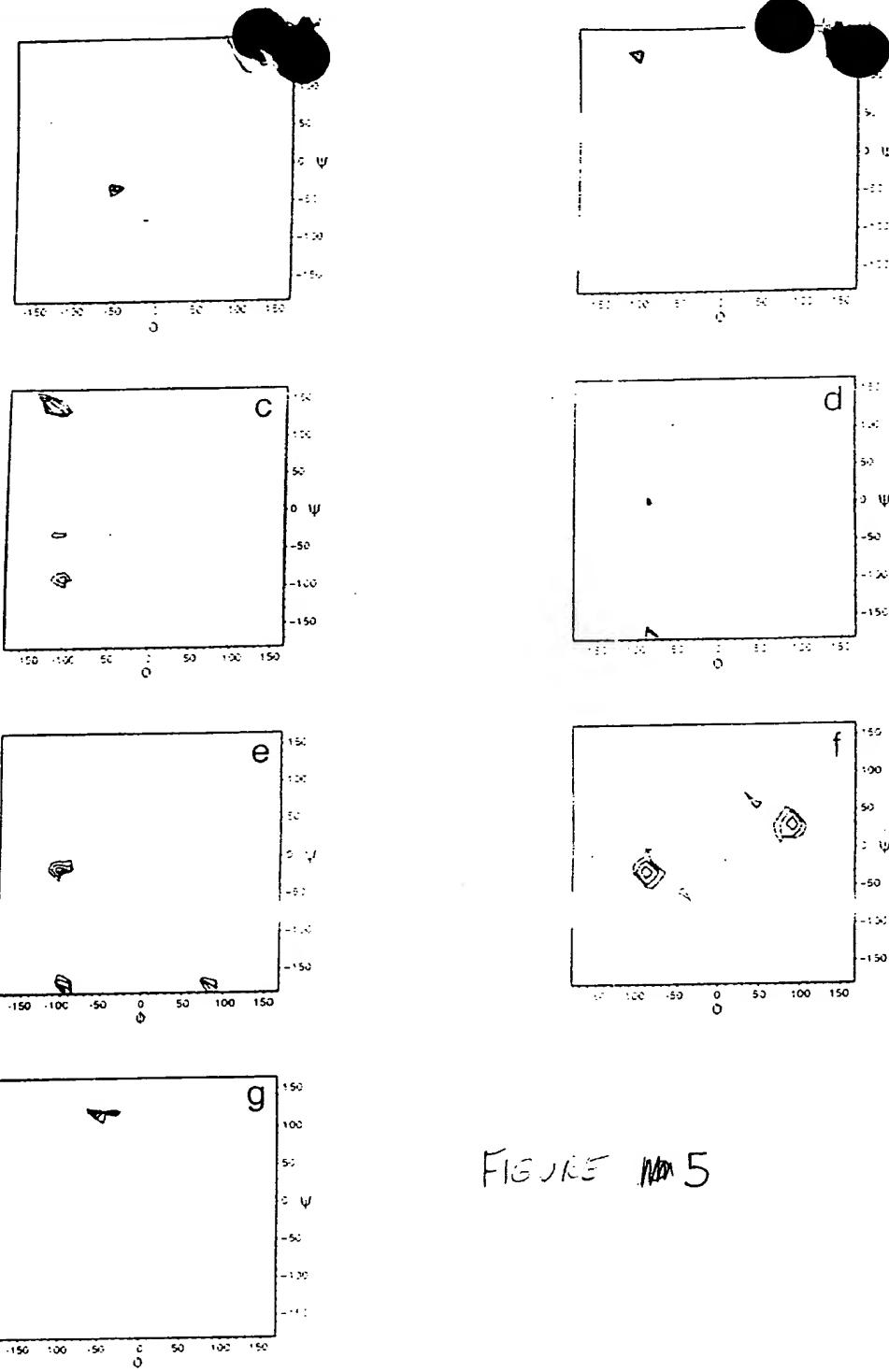


FIGURE NO 5

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Figure 5 of 13

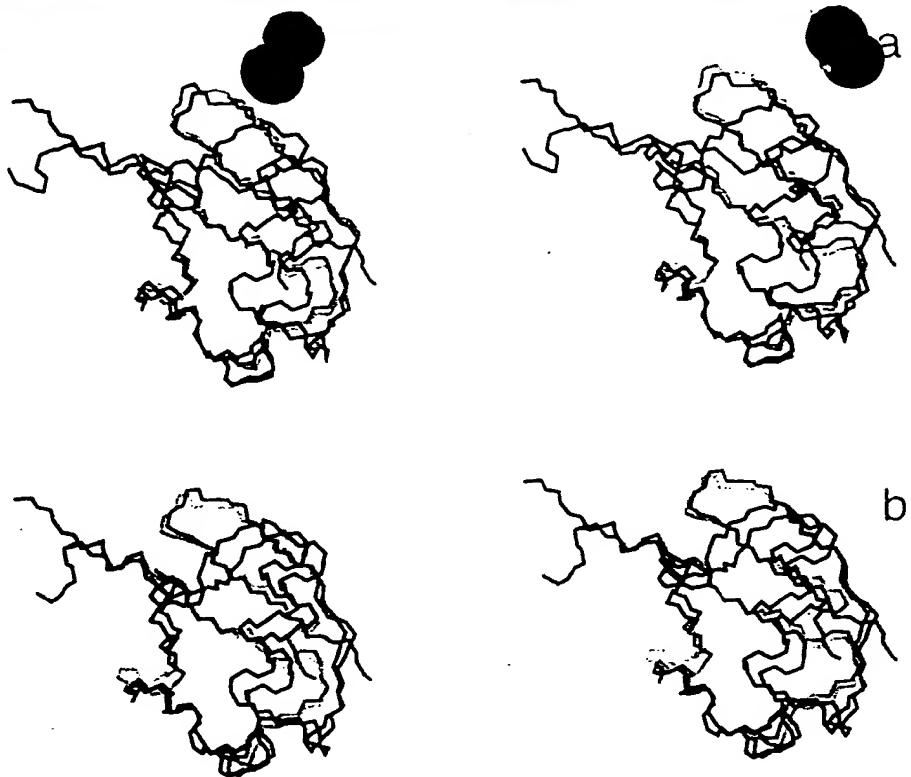


FIGURE 6

09933020 - 102204

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Atty. Dkt. No. 1496-205  
Figure 6 of 13

## FIGURE 7

Generate Linear  
amino-acid chain

Calculate  $\phi, \psi$  angles  
for each peptide pair  
using experimental  
residual dipolar couplings

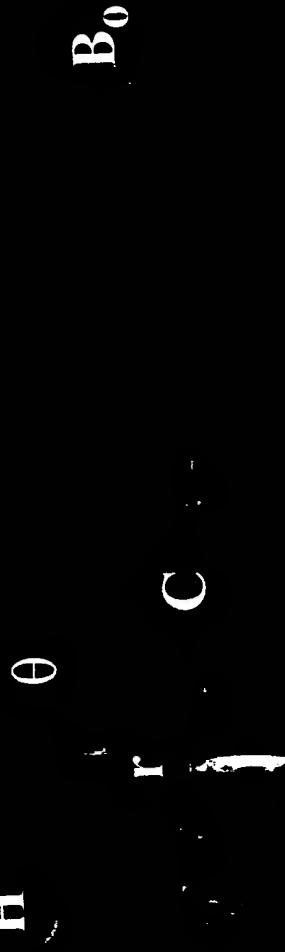
Fold Linear sequence  
with dihedral angle  
and backbone NOE  
restraints

Refine structure  
using NOE and  
dipolar coupling  
restraints

102201 "D9960

FIGURE 8

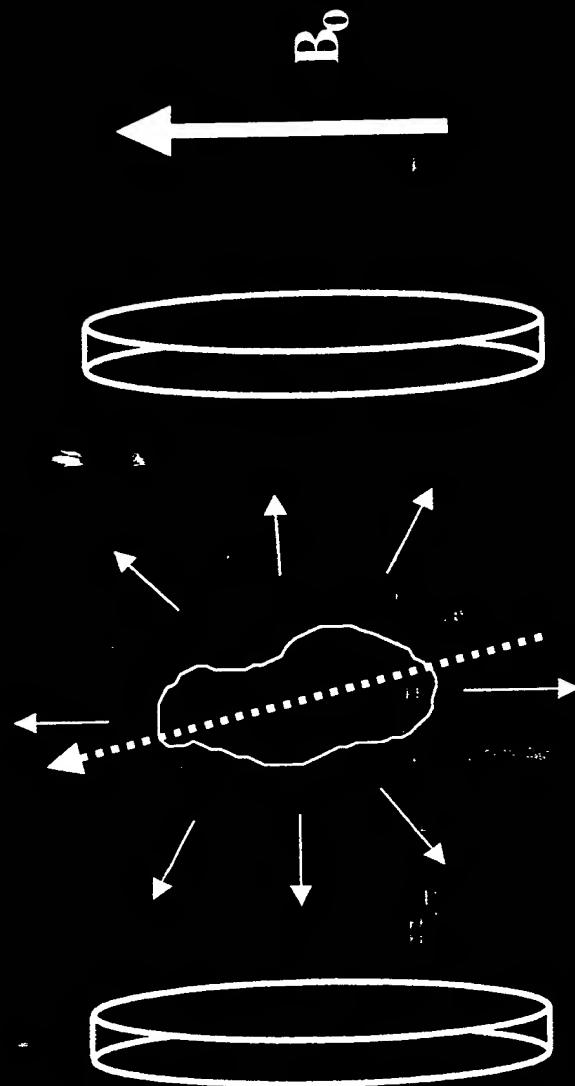
## Dipolar Couplings - Powerful Structural Constraints



$$D \propto (3 \cos^2 \theta - 1) / r^3$$

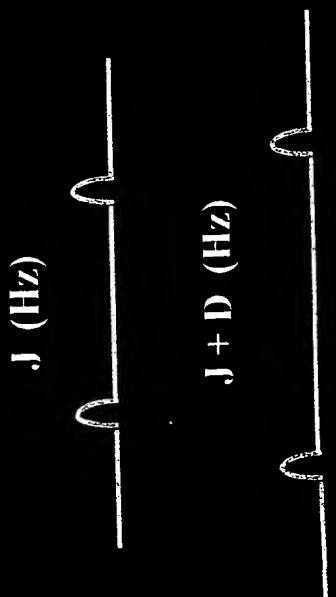


# Measurement of Dipolar Couplings Requires a Weakly Aligned Molecule



Phospholipid Bicelles

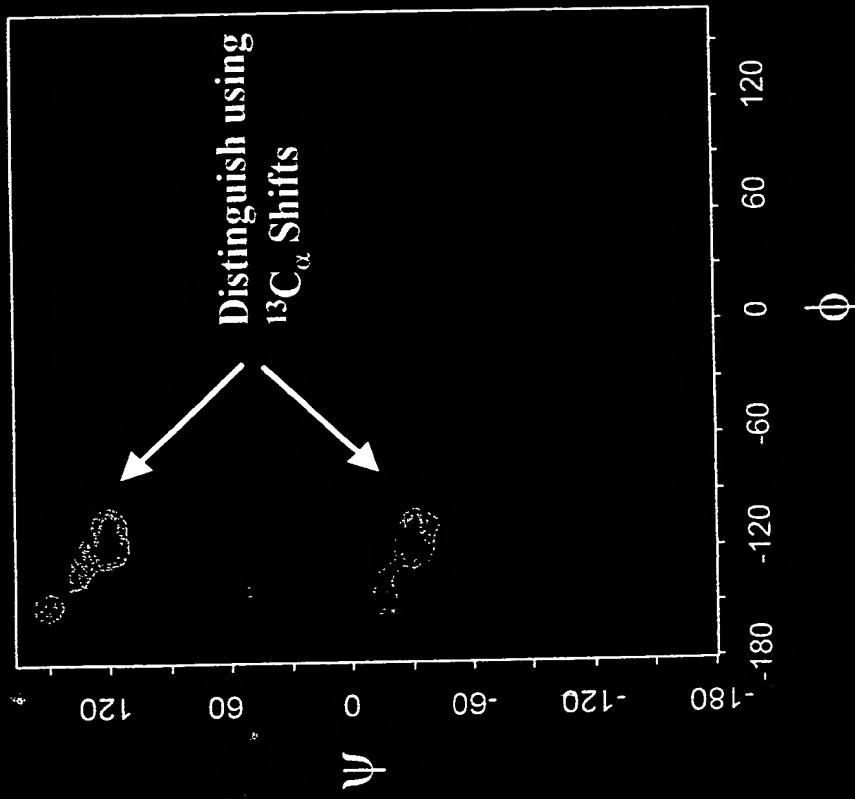
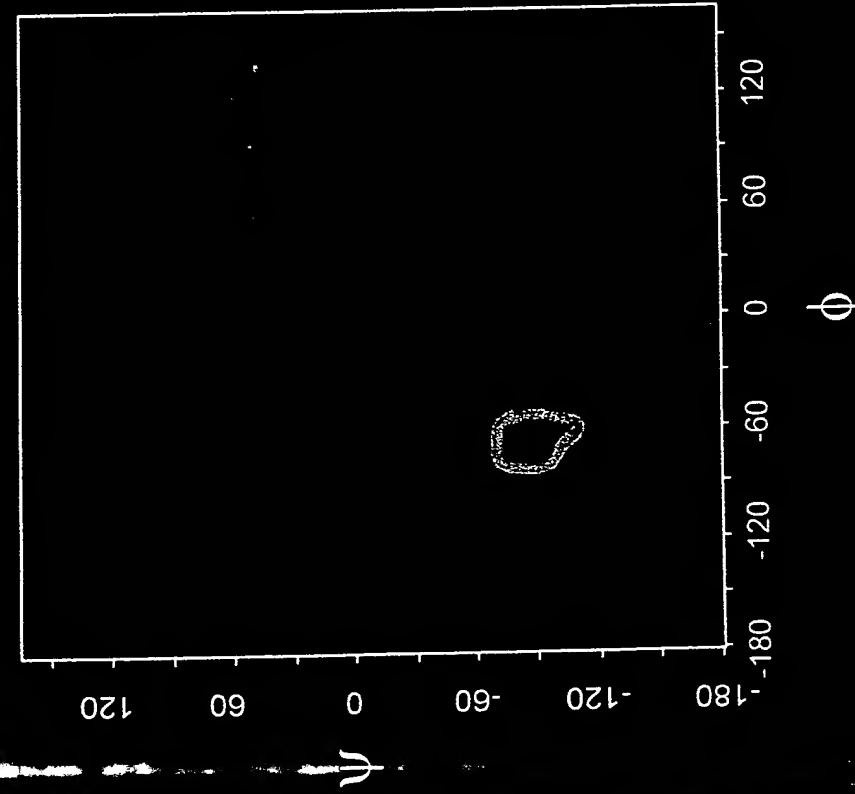
22° C: Isotropic (no alignment)  
35° C: LC Phase (alignment)



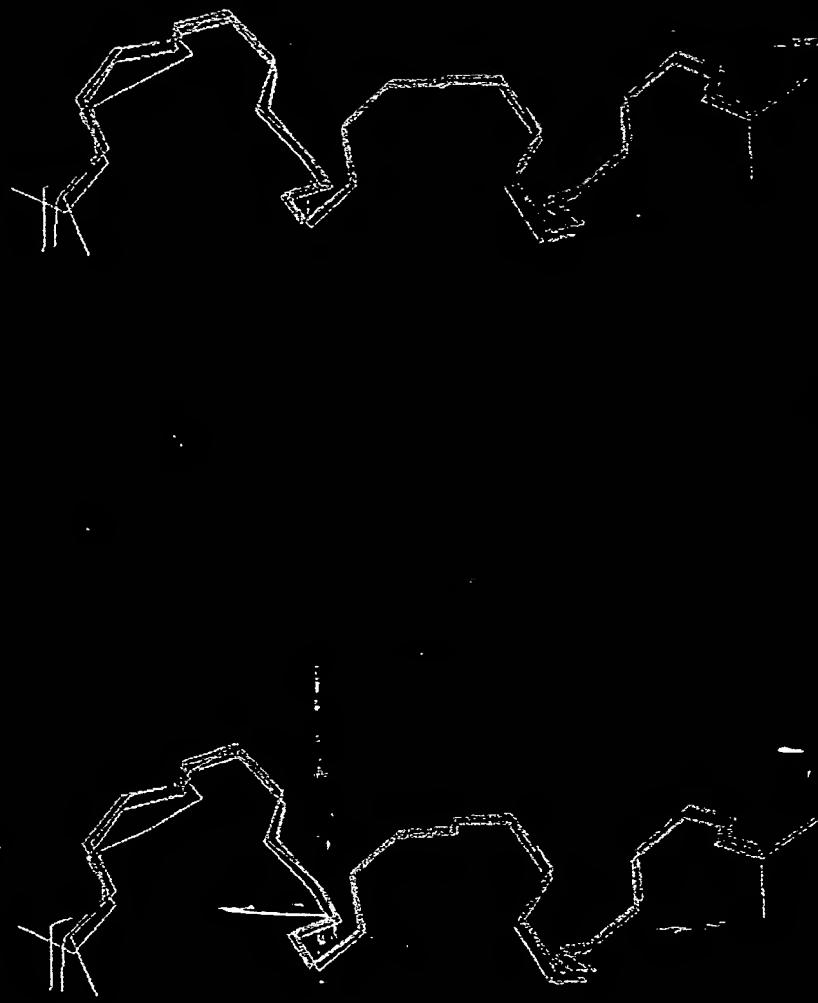
# $\phi, \psi$ Mapping Using Residual Dipolar Couplings

Val 26

Ile 33

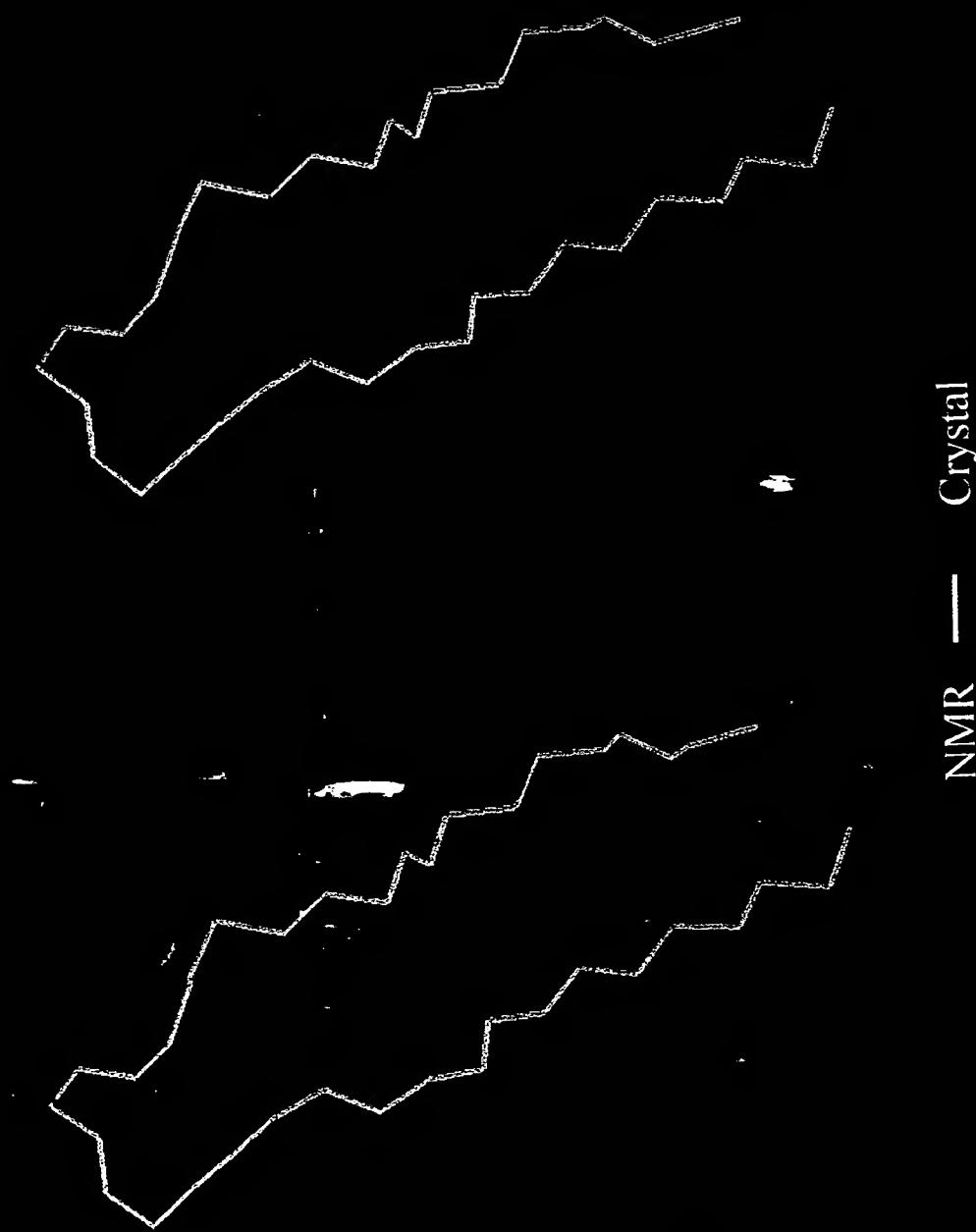


NMR vs. Crystal Structure of  $\alpha$ -helix (24-34) Ubiquitin



NMR — Crystal

FIGURE 12  
NMR vs. Crystal Structure of  $\beta$ -sheet (3-15) Ubiquitin



# Crystal Structure vs. NMR Global Fold - Ubiquitin

FIGURE 13

